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NAVAL WEAPONS STATION, YORKTOWN, VIRGINIA 23691

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Naval Explosives Development Engineering Department

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20. ABSTRACT

A previous technical report described a simple empirical relationship between detonation velocity at theoretical maximum density and a factor, F, that is dependent solely upon chemical composition and structure. The explosives ranged from nitro-aromatics, cyclic and linear nitramines, nitrate esters and nitro-nitrato aliphatics to zero hydrogen explosives, carbonless explosives and hydrogen rich explosives. Minor modifications have been made to the equations presented in that report, including a correction factor for liquid explosives, that have resulted in an improved predictive model in which: 95% of the predicted detonation velocities lie within 5% of experimental, the absolute error for 64 explosives is ± 2.3%; and the correlation coefficient for the linear regression relationship is > 0.96.

F O R E W O R D

1. This is an addendum report to NWSY TR 78-3 documenting the postulate that a simple, empirical linear relationship exists between detonation velocity and a factor, F, that is dependent solely upon the chemical composition and structure for a gamut of explosives, with a correction factor to be used for liquid explosives.

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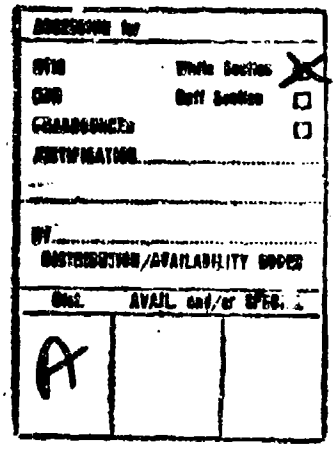

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PREDICTING HIGH EXPLOSIVE DETONATION VELOCITIES FROM THEIR COMPOSITION AND STRUCTURE (II)

In a previous report[1] it was shown that a simple, empirical linear relationship existed between detonation velocity for ideal explosives at theoretical maximum density and a factor, F, dependent solely upon chemical composition and structure. At that time, it was also noted that the calculated detonation velocities for tetranitromethane (TNM) and TNM/nitromethane (NM) mixtures did not fit the proposed model despite their known ideality and that liquid explosives in general calculated to anomalously higher detonation velocities than measured.

It should now be added that if there is a reasonable expectation that a given explosive will be a liquid, a further simple correction can be made in calculating F which substantially reduces the error between predicted and observed detonation velocities.

This revised equation for calculating F is

$$(1)\quad F = \left[100 \times \frac{n(O) + n(N) - \frac{n(H)}{2n(O)} + \frac{A}{3} - \frac{n(B)}{1.75} - \frac{n(C)}{2.5} - \frac{n(\quad)}{4} - \quad E)}{MW}\right] - G$$

where G = 0.4 for liquid explosives, for solid explosives G = 0
A = 1 if the compound is aromatic, otherwise A = 0

and where, as before, for one mole of the composition:

n(O) = number of oxygen atoms
n(N) = number of nitrogen atoms
n(H) = number of hydrogen atoms
n(B) = number of oxygen atoms in excess of those already available to form CO_2 and H_2O

[1]Lewis R. Rothstein and Robert Petersen, NWSY TR 78-3, *Predicting High Explosive Detonation Velocities From Their Composition and Structure*, Sep 1978.

n(C) = number of oxygen atoms doubly bonded directly to carbon as in carbonyl $\overset{|}{C} = O$

n(D) = number of oxygen atoms singly bonded directly to carbon as in a $\overset{|}{C} - O - R$ linkage where R can equal -H, $-NH_4$, -C, etc.

n(E) = number of nitrato groups existing either in a nitrate ester configuration or as a nitric acid salt such as hydrazine mononitrate.

Minor changes to the A, B, C and E fractions have been made over those originally published. Thus, where F previously was reported as

$$100 \times \frac{n(O) + n(N) - \frac{n(H)}{2n(O)} + \frac{n(A)}{4} - \frac{n(B)}{2} - \frac{n(C)}{2} - \frac{n(D)}{4} - \frac{n(E)}{4}}{MW},$$

the principal changes are that: the aromaticity correction factor, (A), is not based, as before, on the number of aromatic rings present but merely upon whether or not the compound is aromatic; additionally, the correction for oxygen in excess of that required to form CO_2 and H_2O, (B), is weighted more heavily, whereas carbonyl oxygen, (C), and nitrato, (E), corrections are de-emphasized slightly. These modifications were made arbitrarily to further improve the correlation coefficient of the linear regression plot of D' experimental versus F.

Molecular weights and atomic compositions for composited explosives were derived respectively from the sum of the weighted average molecular weights and the weighted average sums of each elemental mole fraction as previously described.[2]

Table I lists the experimental detonation velocities previously reported[3] and the detonation velocities predicted from the newly generated linear regression equation

(2) $$F = 0.55\ D' + 0.26$$

or

(3) $$D' = \frac{F - 0.26}{0.55}$$

where, as before, D' is the detonation velocity at theoretical maximum density in millimeters per microsecond (mm/μsec).

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[2] *Ibid.*, Appendix, p. 13.
[3] *Ibid.*, Tables I and II, pp. 6-9.

Substantial improvements in predicted versus experimental D' values are apparent over those previously reported.[4]

- The absolute error for all 64 data points is now ± 2.3% versus 2.8%.
- Sixty-one of sixty-four calculated D' values, 95%, lie within 5% of the experimentally reported values.
- Sixty-three of sixty-four D' values, 98%, lie within 7% of experimental.
- Only one value, NM, is discrepant by -13%.
- The correlation coefficient for the linear regression plot of all data resulting in Eq. (3) is >0.96.
- For the liquid explosives, the percent error between calculated and experimental D' values determined with and without the 0.4 correction factor are as follows:

Explosive:	NIBTN	TNM	TNM/NM	NG	EGDN	NM
From NWSY TR 78-3[4] (w/o liquid correction):	+5%	+20%	+26%	+6%	+11%	0%
From Eqs. (1) and (3):	-1%	+3%	+4%	-3%	+3%	-13%

No attempt has been made to reconcile this basically empirical relationship to more formal theories. Investigators such as Martin and Yallop[5] earlier tried to weight oxygen balance and the strength of the type bonds with detonation velocity. However, Price[6] showed shortly thereafter that their treatment had only limited applicability. More recent investigations[7 8] appear to be merely variations of the theme first introduced by Kamlet, et al.,[9 10 11 12] namely where fairly

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[4] *Ibid.*, pp. 6-7.
[5] A.R. Martin and H.J. Yallop, Trans. Faraday Soc 54 257 (1958).
[6] D. Price, Chem. Rev. 59 801 (1959).
[7] I.N. Aizenstadt, translated from Fizika Goreniyva, Vol 12, No. 5, pp 754-8, Sep-Oct 1976, copy written by Plenum Publishing Corp., New York, NY.
[8] V.I. Pepekin and Yu. A. Lebedev, DOKLADY AKADEMII NAVK, Vol 234, No. 6 (1977), Consultants Bur. Translation, *Ibid.*, p. 460.
[9] M.J. Kamlet and H. Hurwitz, J. Chem. Phys. 48 3690 (1968).
[10] M.J. Kamlet and C. Dickinson, J. Chem. Phys. 48 43 (1968).
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[12] M.J. Kamlet and S.J. Jacobs, J. Chem. Phys. 48 23 (1968).

simple relationships between heats of formations of chosen detonation products, explosive density, ρ_0, and the sought for detonation velocity were demonstrated. It was shown earlier that at least one of these later treatments, that of Aizenstadt, was inferior to both Kamlet's and that presented in NWSY TR 78-3.[13]

Since the even simpler relationship presented here and in NWSY TR 78-3[1] is based exclusively upon composition and structure - (that is if one allows for predictive knowledge of whether or not an explosive is a liquid or a solid) - it is concluded, inescapably, that this compositional/structural relationship, albeit highly empirical, must be more than casually correlatable to the more fundamental thermochemical (ΔH_f) and physical (ρ_0) factors just mentioned. However, since any empirical relationship may be found wanting with increased data availability, additional experimental detonation velocity and theoretical maximum density data would be welcomed by the authors for further testing of the relationships presented here. Of particular interest would be detonation velocity data on the many heterocyclic nitroaromatics that have been synthesized in recent years but for which no detonation velocity data has been published.

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[13] *Op cit.*, Addendum, pp. 14-15.

TABLE I. PREDICTED DETONATION VELOCITIES

No.	Xpl	TMD (g/cc)	Elemental composition				Mol wt	Exptl D' (mm/μsec)	Factor F	Calc'd D' (mm/μsec)	% error
			C	H	N	O					
1	HNB	2+	6	-	6	12	348	9.50	5.27	9.11	-4
2	SORGUYL	2.01	4	2	8	10	322	9.15	5.13	8.85	-3
3	HMX	1.90	4	8	8	8	296	9.14	5.24	9.05	-1
4	BTNEU	1.86	5	6	8	13	386	9.00	5.28	9.13	+1
5	9404	1.87	4.20	8.26	7.73	8.09	296	8.89	5.17	8.93	+1
6	RDX	1.83	3	6	6	6	222	8.85	5.18	8.95	+1
7	BTNEN	1.96	4	4	8	14	388	8.85	5.04	8.69	-2
8	HN	1.64	0	5	3	3	95	8.69	4.88	8.40	-3
9	BTF	1.90	6	-	6	6	252	8.61	4.89	8.42	-2
10	9011	1.80	5.12	9.41	7.55	7.73	296	8.59	4.96	8.55	-1
11	OCTOL	1.83	4.94	7.14	6.53	7.44	278	8.54	4.88	8.40	-2
12	9010	1.82	3.35	5.86	5.86	5.86	222	8.49	5.05	8.71	+3
13	COMP C-4	1.59(?)	4.02	7.82	5.44	5.55	222	8.04	4.65	7.98	-1
14	CYCLOTOL	1.77	3.96	5.73	5.24	5.98	223	8.33	4.85	8.35	0
15	9205	1.72	4.04	6.94	5.50	5.55	222	8.32	4.72	8.11	-3
16	TNETB	1.78	6	6	6	14	386	8.30	4.97	8.56	+3
17	PETN	1.77	5	8	4	12	316	8.29	4.71	8.09	-2
18	MHN	1.73	6	8	6	18	452	8.26	4.70	8.07	-2
19	EDNA	1.71	2	6	4	4	150	8.23	4.83	8.31	+1
20	NQ	1.72	1	4	4	2	104	8.16	4.81	8.27	+1
21	DINGU	1.94	4	4	6	6	232	8.15	4.69	8.05	-1
22	DNPN	1.73	6	10	6	10	326	8.10	4.75	8.16	+1
23	COMP B-3	1.74	4.53	5.56	4.78	5.96	221	8.05	4.71	8.09	+1
24	DINA	1.67	4	8	4	8	240	8.00	4.63	7.95	-1
25	TATB	1.94	6	6	6	6	258	7.94	4.59	7.87	-1
26	TETRYL	1.73	7	5	5	8	287	7.91	4.54	7.78	-2
27	NIBTN	1.64	4	6	4	11	286	7.86	4.54	7.78	-1
28	K-SALT	1.57(?)	3	6	6	3	174	7.80	4.60	7.89	+1
29	TPEON	1.58	15	24	8	26	732	7.71	4.29	7.34	-5
30	NG	1.60	3	5	3	9	227	7.70	4.35	7.44	-3
31	EDD	1.60	2	10	4	6	186	7.69	4.71	8.09	+5
32	DATB	1.84	6	5	5	6	243	7.67	4.49	7.69	0
33	HNAB	1.77	12	4	8	12	452	7.65	4.40	7.53	-2
34	PETRIN	1.54(?)	5	9	3	10	271	7.64	4.32	7.38	-3

TABLE I. PREDICTED DETONATION VELOCITIES (cont'd)

No.	Xpl	TMD (g/cc)	Elemental composition				Mol wt	Exptl D' (mm/μsec)	Factor F	Calc'd D' (mm/μsec)	% error
			C	H	N	O					
35	DNPTB	1.68	7	9	5	12	355	7.63	4.50	7.71	+1
36	TNPON	1.68(?)	8	6	4	10	318	7.60	4.27	7.29	-4
37	DPEHN	1.63	10	16	6	19	524	7.53	4.41	7.55	0
38	PIC ACID	1.76	6	3	3	7	229	7.50	4.31	7.36	-2
39	DIPAM	1.79	12	6	8	12	454	7.49	4.35	7.44	-1
40	TNA	1.76	6	4	4	6	228	7.42	4.38	7.49	+1
41	XPL D	1.72	6	6	4	7	246	7.36	4.33	7.40	+1
42	GTNB	1.63	10	12	6	16	472	7.34	4.31	7.36	0
43	EGDN	1.48(?)	2	4	2	6	152	7.30	4.38	7.49	+3
44	TNB	1.64(?)	6	3	3	6	213	7.27	4.26	7.27	0
45	TACOT	1.85	12	4	8	8	388	7.25	4.14	7.05	-3
46	HNDP	1.64(?)	12	5	7	12	439	7.20	4.36	7.45	+4
47	HNDPO	1.70(?)	12	4	6	13	440	7.18	4.30	7.35	+2
48	HNS	1.74	14	6	6	12	450	7.12	4.02	6.84	-4
49	DNDMOA	1.52(?)	4	6	4	6	206	7.10	4.22	7.20	+1
50	FIVONITE	1.59(?)	9	12	4	13	384	7.04	3.99	6.78	-4
51	DIAZ	1.63	6	2	4	5	210	7.00	4.23	7.22	+3
52	HNDS*	1.65(?)	12	4	6	13	456	7.00	4.15	7.07	+1
53	TNT	1.65	7	5	3	6	227	6.96	3.93	6.67	-4
54	NM/TNM**	...	1.00	2.40	1.60	3.20	88	6.88	4.20	7.16	+4
55	TNC	1.68(?)	7	5	3	7	243	6.85	4.00	6.80	-1
56	DNPEN	1.60(?)	8	7	3	8	273	6.80	3.83	6.49	-5
57	ET PIC	1.60(?)	8	7	3	7	257	6.80	3.73	6.31	-7
58	TNAN	1.61(?)	7	5	3	7	243	6.80	4.00	6.80	0
59	DEGN	1.38	4	8	2	7	196	6.76	3.97	6.75	0
60	TNM	1.65	1	0	4	8	196	6.55	3.97	6.75	+3
61	TMPTN	1.50(?)	6	11	3	9	269	6.44	4.01	6.82	+6
62	DNPF	1.60	10	12	4	12	380	6.38	3.74	6.33	-1
63	NM	1.16	1	3	1	2	61	6.32	3.29	5.51	-13
64	TNN	...	10	5	3	6	263	6.00	3.39	5.69	-5

*Sulfur atom treated as an oxygen.
**1:025 mole ratio.

Note: (?) indicates that the reference value given is at the experimental condition and TMD data is not listed.

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